



chain nodes :

15 16 19 20 21 22

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14

chain bonds :

2-19 7-15 10-16 12-20 19-22 20-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 13-14

exact/norm bonds :

1-2 1-6 2-3 2-19 3-4 4-5 5-6 5-7 6-10 7-8 7-15 8-9 8-11 9-10 9-14 10-16 11-12  
12-13 12-20 13-14 19-22 20-21

G1:Br,F,I,CH3,Et,n-Pr,s-Bu,CF2,CN,C,S,Si

G2:C,N

G3:C,I,F,NO2,S,N,Si,OH,SH,MeO,EtO

Match level :

1:Atom 2:Atom 3:CLASS 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS